

# The CCA ISIC and You (aka CCTTSS)

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Co-Investigators:

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http://www.cca-forum.org/ccttss

March 2003 PI Meeting





















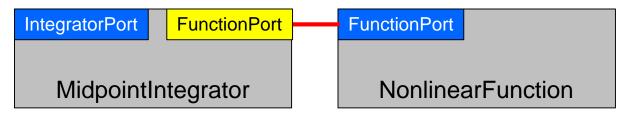
### **Outline**

- CCA Components: what are they?
- Working with the CCA
  - Software
  - Tutorials
  - Getting help: CCA adepts and community
- Future of the CCA



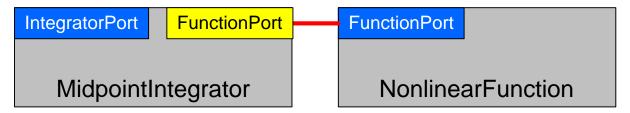
## What are components, frameworks?

- No universally accepted definition...yet
  - My working def'n: software that is composable
  - Framework is everything that isn't a component
- Interacts with the outside world only through well-defined interfaces
  - Implementation is opaque to the outside world
- Can be composed with other components
  - "Plug and play" model to build applications
  - Composition based on these interfaces





## **Ports: Connections Interface Exchange**

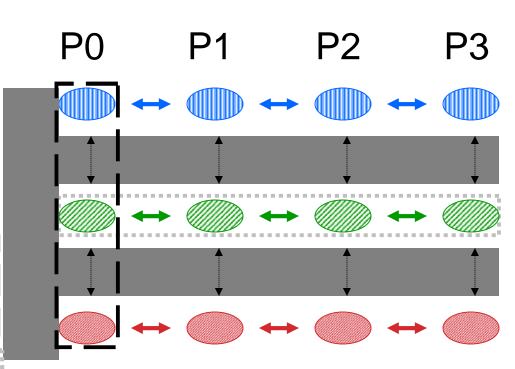


- Components interact through well-defined interfaces, or ports
  - In OO languages, a port is a virtual class or interface
  - In Fortran, a port is a bunch of subroutines or a module
- Components may provide ports implement the class or subroutines of the port
- Components may use ports call methods or subroutines in the port
- Links denote a caller/callee relationship, not dataflow!
  - e.g., FunctionPort could contain: evaluate(in Arg, out Result)



# Framework Stays "Out of the Way" of Component Parallelism

- Single component multiple data (SCMD) model is component analog of widely used SPMD model
- Each process loaded with the same set of components wired the same way
- Different components in same process "talk to each" other via ports and the framework
- Same component in different processes talk to each other through their favorite communications layer (i.e. MPI, PVM, GA)



Components: Blue, Green, Red

Framework: Gray

MCMD/MPMD also supported



# **Working with CCA**

- The CCA components are easy to build
  - Designed to easily import existing code into components
  - Reversible you don't "lose" the original code
- Significant components available to download
  - Buildable code right now
  - RPMs real soon now
- Tutorials are hands on and no nonsense
  - You will be able to build a component
  - Tutorials are usually conducted in and around CCA mtg's.
  - Copies of all tutorial presentations are on the web



# Making your code CCA compliant in 2 easy steps

- 1. Create a single method, function, or subroutine in C++, C, or Fortran
  - C++ SIDL rendering:void setServices(Services svc) { /\*...\*/
- 2. There isn't a "2".
- This won't make a very interesting component.

More interesting component: put more code here



## CCA leaves your code alone

 Everything that makes your component a component is right here:

```
void setServices(Services svc) { /*...*/}
```

- The rest of the code is yours.
- The really hard part we have yet to talk about: carefully define what functionality your component
  - Provides to the outside world
  - Uses from the outside world



## **CCA Software: Component Inventory**

#### Services and Performance

- Ccaffeine SNL Services for parameter ports, connections between SIDL and classic ports, MPI access, etc.
- Performance Component –
   Oregon/LANL/SNL classic & SIDL –
   Measurement capabiliites for components

#### Data Management, Meshing, and Discretization

- Global Array Component PNNL classic & SIDL – Multidimensonal dense distributed arrays
- TSTTMesh ANL/SNL classic Unstructured mesh management
- FEMDiscretization ANL/SNL classic Finite element discretization
- GraceComponent SNL classic Parallel structured adaptive mesh refinement

#### Integration and Optimization

- CvodeComponent LLNL (TOPS) classic Implicit ODE integrators
- TAOSolver ANL SIDL Solvers for constrained and unconstrained optimization

- Parallel Data Description, Redistribution, and Visualization
  - DistArrayDescriptorFactory ORNL

     classic Uniform means for
     describing dense multi-dimensional
     arrays
  - CumulvsMxN ORNL classic "MxN" parallel data redistribution
  - VizProxy ORNL classic –
    Companion "MxN" endpoint for
    passing data to front-end viewers for
    graphical rendering

#### Scientific Applications

- Chemistry components SIDL PNNL/SNL – electronic structure components based on NWChem and MPQC
- Combustion components classic SNL – based on GrACEComponent and physical/chemical models

RPM coordinator: B. Allan (SNL)



### The CCA Tutorial

## CCA Forum Tutorial Working Group

Rob Armstrong (SNL), David Bernholdt (ORNL, chair), Lori Freitag Diachin (SNL), Wael Elwasif (ORNL), Dan Katz (JPL), Jim Kohl (ORNL), Gary Kumfert (LLNL), Lois Curfman McInnes (ANL), Boyana Norris (ANL), Craig Rasmussen (LANL), Jaideep Ray (SNL), Torsten Wilde (ORNL)

## Highlights:

- CCA Concepts
- A Simple Component Example
- Language Interoperability using Babel
- Writing CCA Components
- More Complex Component-Based Applications
- CCA Status and Plans



### **Tutorial Presentations**

Jan 2002 CCA Forum Mtg Santa	Fe, NM
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Apr 2002 CCA Forum Mtg Townsend, TN

Jun 2002 CCA Forum Mtg ANL

Sep 2002 ACTS Collection LBL

Workshop

Oct 2002 CCA Forum Mtg Half Moon Bay, CA

Oct 2002 LACSI Symposium Santa Fe, NM

Nov 2002 SC2002 Baltimore, MD

Jan 2003 CCA Forum Mtg Pasadena, CA



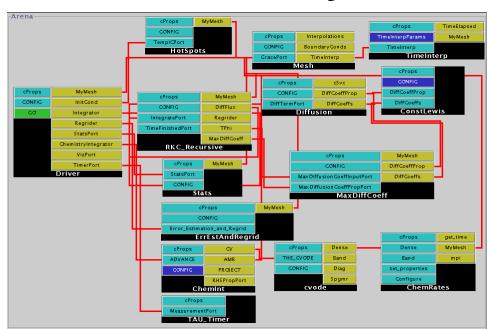
## Getting help with CCA technology

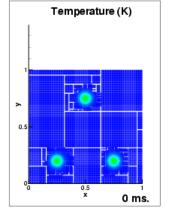
- Write to: cca-pi@cca-forum.org
- Usually adopters of CCA have a CCTTSS liaison assigned to them
- Online manuals, tutorials:
   http://www.cca-forum.org

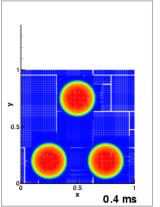


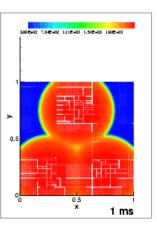
## Reacting Flow Software "Facility"

- A Computational Facility for Reacting Flow Science (CFRFS), SciDAC application center, PI: H. Najm
- Epitome of componentized applications
  - There is no one application, but a component "facility"











### **Future of CCA**

- Current big adopters are:
  - Combustion (CFRFS)
  - Quantum Chemistry
- This year
  - big climate apps push
  - a couple approaches for Fortran components exist
    - climate and fusion early adopters
- More and better components
  - structured, unstructured meshes (APDEC, TSTT)
  - MxN, parallel IO
  - refinements of existing frameworks and components



# CCA will help you componentize your code

- Converting your code is easy and reversible
  - Creating interfaces is the hard part
- Significant and useful software in the form of frameworks and components are available
- Much documentation and tutorials available



# **CCA Impact Outside of SciDAC**

Climate prototype (Courtesy Shujia Zhou, ESMF)

